Open Day at HITS: AI for weather, viruses and the Universe

On 13 July 2024, HITS opened its doors to the public again. The program titled "Weather, viruses and the universe - exploring the role of AI in tomorrow's world," included hands-on stations and scientific talks (not only) about Artificial Intelligence, showcasing the research conducted at the institute.

More than 500 visitors came to the HITS campus where they learned in easy-to-understand presentations that black holes are anything but silent, why you shouldn't blindly trust large language models such as ChatGPT and how computer simulations make work easier for biologists and chemists.

There were also guided garden tours and several hands-on stations where you could put your skills to the test by building dams, sorting maps and training an AI. Highlights for the younger guests included face painting and a photo station with a green screen, where everyone had lots of fun and could take home a printout to remember the day at HITS.

HEIDELBERG LAUREATE FORUM

22–27 September 2024
HITS at the Heidelberg Laureate Forum

HITS

Frauke Gräter appointed Max Planck Director

Frauke Gräter, long-standing head of the "Molecular Biomechanics" group, has been appointed new director at the Max Planck Institute for Polymer Research (MPI-P) in Mainz where she will contribute her expertise and experience in mechanobiology to the area of "soft matter". After a six months' transition phase, Frauke Gräter will leave at the end of the year. "We see the appointment as confirmation of Frauke's outstanding achievements, but also as a success for us as a research institute," says HITS Scientific Director **Tilmann Gneiting**. "We are delighted that the concept of our founder Klaus Tschira has once again paid off: bringing brilliant young researchers to the institute, giving them the greatest possible freedom to conduct their research, but also giving them responsibility and thus enabling them to pursue a scientific career up to top positions."

In 2009, Frauke Gräter came to HITS (then EML Research) at the age of 32 to do research in molecular biomechanics. As HITS Scientific Director in 2021/2022, she pushed the interdisciplinary collaboration between the HITS research groups.

Moreover, she is a co-founder of the SIMPLAIX initiative on bridging scales from molecules to molecular materials by multiscale simulation and machine learning.

New employees and visiting scientists

PhD students:	Souvik Banerjee (NLP), Johannes Hengstler (CME), Kristián Vitovský (PSO)
Master student:	Vijayalakshmi Vijayakumaran Nair (PSO)
Visiting scientists:	Guillermo Cabrera-Vives (Klaus Tschira Guest Professor, Universidad de Concepción, Chile), Christina Fakiola (PSO, Heidelberg University), Damien Gagnier (PSO, Karls-Universität Prag, Czech Republic), Evans Kojo Owusu (PSO, UNSW Canberra, Australia), Ashley Ruiter (PSO, UNSW Canberra, Australia), Ivo Seitenzahl (PSO, UNSW Canberra, Australia)

HITS groups (09/2024): *Astroinformatics (AIN), Computational Molecular Evolution (CME), Computational Statistics (CST), Data Mining and Uncertainty Quantification (DMQ), Machine Learning and Artificial Intelligence (MLI), Molecular Biomechanics (MBM), Molecular and Cellular Modeling (MCM), Natural Language Processing (NLP), Physics of Stellar Objects (PSO), Scientific Databases and Visualization (SDBV), Stellar Evolution Theory (SET), Theory and Observations of Stars (TOS).*

HITSters

Digital babies created to improve infant healthcare

An international team of researchers at HITS, Heidelberg University Hospital, and the University of Galway, Ireland, have created so-called "digital twins" to better understand infants' health in their critical first 180 days of life. The team created 360 advanced computer models that simulate the unique metabolic processes of each baby. The digital babies are the first sex-specific computational whole-body models representing newborn and infant metabolism with 26 organs, six cell types, and more than 80,000 metabolic reactions. The study was published in the journal "Cell Metabolism" in June this year.

Searching for clues in infant metabolism

For years, medical research has been looking into individually tailored medication and therapies with the aim of personalized healthcare. This involves the use of "digital twins", which use algorithms and data to simulate metabolism, while taking into account the dynamics of individual organs. These "digital twins" already existed for adults. However, although the metabolism of babies differs considerably from that of adults, such models have been lacking for infants until now.

Lead author **Elaine Zaunseder** from the Data Mining and Uncertainty Quantification (DMQ) group explains: "Babies are not little adults – they have unique metabolic features that allow them to develop and grow up healthy." Newborns have considerably less mass in relation to their body surface than adults and therefore need more energy to regulate their body temperature. However, they cannot shiver in the first six months of life. Metabolic processes ensure that the infant stays warm.

Mathematics behind medicine – towards individualized therapies

An essential part of the team's research was to advance precision medicine using computational modeling. Computer-assisted modeling of infants is seen by researchers as highly promising for the future, as it not only deepens the overall understanding of infant metabolism, but also creates opportunities to improve the diagnosis and treatment of diseases in the first days of an infant's life.

Zaunseder E et al: Personalized metabolic whole-body models for newborns and infants predict growth and biomarkers of inherited metabolic diseases. Cell Metabolism, 4 June 2024. (DOI: 10.1016/j.cmet.2024.05.006)

Research

Mike Lau, PostDoc and Croucher Research Fellow

Mike Lau, PostDoc and Croucher Research Fellow, has been part of the Physics of Stellar Objects Group (PSO) since September 2023. In a video interview for the institute's social media channels, he explains why he decided to come to HITS after his PhD and that common envelope evolution can be much more complicated than initially anticipated.

You've been at HITS for almost a year now. What has been your most memorable experience so far?
My most memorable experience at HITS was actually when I first visited around six months ago, before I started as a research fellow. I was finishing my PhD and was deciding where to take the next stage of my academic career. I was very pleasantly surprised by the nice environment I saw at the institute and had very friendly and insightful interactions with scientists here. So, I've decided to come to HITS in the end.

To many people astrophysics is literally "rocket science". How would you describe your research in simple terms?
My research looks at what happens when one giant star swallows another star, forming what's called a common envelope. We think that stars can survive this phase. In this process, much of the material that makes up the big giant star can go away and leave behind the two stars in a much smaller orbit with each other. We believe this is required to explain a lot of the objects we see in the night sky.

The main area of your scientific research is the interactions in stellar multiples and binary stellar evolution. You planned on continuing your research in the common-envelope evolution with 3D hydrodynamic simulations. Have you been able to make progress in this field?
We are currently running these simulations on computer clusters and are analyzing the outcome. The emerging picture from our group seems to be that common envelope evolution is much more complicated than we initially anticipated. It probably involves many other phases and interactions after the main common envelope.

You completed your undergraduate education at the University of Oxford, UK, and did your PhD at the Monash University in Melbourne, Australia. You already have quite an impressive career path. What is it that drives you as a scientist?
Part of why I'm doing all this research is of course because it's very fun and makes use of a lot of the physics that I've learned and that I understand. It's quite a challenge to combine these different physical models to explain things we see in the night sky. Also, I just like to contribute to the humanity's understanding of the universe which is the more noble goal behind all this.

You are originally from Hong Kong. What is it that you miss most about home while living in Germany?
Food and convenience. This is why I usually cook traditional Cantonese food for dinner here in Germany. Back home I would typically go to the mall to buy something I need. I would know exactly which store to go to. It's a bit more challenging here. But I manage to get what I need.

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Pictures: HITS, Gülay Keskin, Heidelberg University Hospital

Beyond the limits

HITS

The Charts

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